

ESD Fundamental/Exploratory Research Program Publications List

2011

Peer-Reviewed Journal Articles, Books, and Book Chapters for 2011

1. Ali, S., M. Stute, T. Torgersen, G. Winckler, and B.M. Kennedy (2011), Helium measurements of pore-fluids obtained from SAFOD drillcore. *Hydrogeology Journal*, 19 (1), 237–247; DOI: 10.1007/s10040-010-0645-6. LBNL-3690E.
2. Armstrong, R., and J. Ajo-Franklin (2011), Investigating biomineralization using synchrotron based x-ray computed microtomography. *Geophysical Research Letters*, 38, L08406; DOI: 10.1029/2011GL046916. LBNL-4754E.
3. Berryman, J.G. (2011), Mechanics of layered anisotropic poroelastic media with applications to effective stress for fluid permeability. *International Journal of Engineering Science*, 49 (1), 122–139; DOI:10.1016/j.ijengsci.2010.06.027). LBNL-3589E.
4. Berryman, J.G. (2011), Bounds and self-consistent estimates for elastic constants of granular polycrystals composed of orthorhombics or crystal with higher symmetries. *Physical Review E*, 83, 046130; DOI:10.1103/PhysRevE.83.046130. LBNL-4411E.
5. Berryman, J.G. (2011), Poroelastic response of orthotropic fractured porous media. *Transport in Porous Media*, DOI: 10.1007/s11242-011-9922-7. LBNL-5254E.
6. Bourg, I.C., and G. Sposito (2011), Molecular dynamics simulations of the electrical double layer on smectite surfaces contacting concentrated mixed electrolyte ($\text{NaCl}-\text{CaCl}_2$) solutions. *Journal of Colloid and Interface Science*, 360, 701–715. LBNL-4934E.
7. Bourg, I.C., and G. Sposito (2011), Ion exchange phenomena. In: *Handbook of Soil Science*, 2nd Edition, P.M. Huang, Y. Li, and M.E. Sumner, eds., Chapter B6, CRC Press, Boca Raton, FL. LBNL-4940E.
8. Commer, M., G.A. Newman, K.H. Williams, and S.S. Hubbard (2011), Three-dimensional induced polarization data inversion for complex resistivity. *Geophysics*, 76 (3), F157–171; DOI:10.1190/1.3560156. LBNL-4759E.
9. DePaolo, D.J. (2011), Surface kinetic model for isotopic and trace element fractionation during precipitation of calcite from aqueous solutions. *Geochimica et Cosmochimica Acta*, 75, 1039–1056; DOI:10.1016/j.gca.2010.11.020. LBNL-4248E.
10. He, G., G. Pan, M. Zhang, and G.A. Waychunas (2011), Coordination structure of adsorbed Zn(II) at water-TiO₂ interfaces. *Environmental Science & Technology*, 45 (5), 1873–1879; DOI: 10.1021/es1035283. LBNL-4274E.
11. Kwon, K.D., K. Refson, S. Bone, R. Qiao, W. Yang, Z. Liu, and G. Sposito (2011), Magnetic ordering in tetragonal FeS: Evidence for strong itinerant spin fluctuations. *Physical Review B*, 83, 064402. LBNL-4983E.
12. Navarre-Sitchler, A., C.I. Steefel, P.B. Sak, and S.L. Brantley, (2011), A reactive-transport model for weathering rind information on basalt. *Geochimica et Cosmochimica Acta*, 75 (23), 7644-7667; DOI: 10.1016/j.gca.2011.09.033.
13. Nielsen, L., J. Druhan, W. Wang, and D.J. DePaolo (2010), Calcium isotopes as tracers of biogeochemical processes. In: *Handbook of Environmental Isotope Geochemistry*,

- Vol I, M. Baskaran, ed., Advances in Isotope Geochemistry, Chapter 7, pp. 105–124; DOI: 10.1007/978-3-642-10637-8_7.
14. Pili, E., B.M. Kennedy, M.E. Conrad, and J.-P. Gratier (2011), Isotopic evidence for the infiltration of mantle and metamorphic CO₂-H₂O fluids from below in faulted rocks from the San Andreas Fault System. *Chemical Geology*, 281 (3-4), 242-252; DOI:10.1016/j.chemgeo.2010.12.011. LBNL-4273E.
 15. Simon, J.I., I.D. Hutcheon, S.B. Simon, J.E.P. Matzel, E.C. Ramon, P.K. Weber, L. Grossman, and D.J. DePaolo (2011), Oxygen isotope variations at the margin of a CAI records circulation within the solar nebula. *Science*, 331, 1175–1178; DOI: 10.1126/science.1197970.
 16. Sung, J., L. Zhang, C. Tian, G.A. Waychunas, and Y.R. Shen (2011), Surface structure of protonated R-plane-sapphire (1-102) studied by sum frequency vibrational spectroscopy. *Journal of American Chemical Society*, 133 (11), 3846–3853; DOI: 10.1021/ja104042u.
 17. Sung, J., G.A. Waychunas, and Y.R. Shen (2011), Surface-induced anisotropic orientations of interfacial ethanol molecules at air/sapphire (1-102) and ethanol/sapphire (1-102) interfaces. *Journal of Physical Chem. Letters*, 2 (14), 1831–1835; DOI: 10.1021/jz2006397.
 18. Sung, J., L. Zhang, C. Tian, Y.R. Shen and G.A. Waychunas (2011), Effect of pH on the Water/a-Al₂O₃ (1-102) interface structure studied by sum-frequency vibrational spectroscopy. *Journal of Physical Chemistry C*, 115 (28), 13887-13893; DOI: 10.1021/jp2046596.
 19. Tokunaga, T. (2011), Physicochemical controls on absorbed water film thickness in unsaturated geological media. *Water Resources Research*, 47, W08514; DOI: 10.1029/2011WR010676. LBNL-4943E.
 20. Vasco, D.W. (2011), On the propagation of a quasi-static disturbance in a heterogeneous, deformable, and porous medium with pressure-dependent properties. *Water Resources Research*, 47, W12523; DOI: 10.1029/2011WR011373. LBNL-5285E.
 21. Vasco, D.W. (2011), On the propagation of a coupled saturation and pressure front. *Water Resources Research*, 47, W03526; DOI:10.1029/2010WR97-865. LBNL-4185E.
 22. Watkins, J.M., D.J. DePaolo, F.J. Ryerson, and B. Peterson (2011), Influence of liquid structure on diffusive isotope separation in molten silicates and aqueous solutions. *Geochimica et Cosmochimica Acta*, 75, 3103–3118. LBNL-5133E.

2010

Peer-Reviewed Journal Articles, Books, and Book Chapters for 2010

1. Aciego, S.M., F. Jourdan, D.J. DePaolo, B.M. Kennedy, P.R. Renne, and K.W.W. Sims (2010), Combined U-Th/He and ⁴⁰Ar/³⁹Ar geochronology of post-shield lavas from the Mauna Kea and Kohala volcanoes, Hawaii. LBNL-3059E. *Geochimica et Cosmochimica Acta*, 74 (5), 1620–1635; DOI:10.1016/j.gca.2009.11.020.

2. Ali, S., M. Stute, T. Torgersen, G. Winckler, and B.M. Kennedy (2010), Helium measurements of pore-fluids obtained from SAFOD drillcore. LBNL-3690E. *Hydrogeology Journal*, DOI:10.1007/s10040-010-0645-6.
3. Aydin, A., and J.G. Berryman (2010), Analysis of the growth of strike-slip faults using effective medium theory. LBNL-3014E. *Journal of Structural Geology*, 32, 1629–1642; DOI:10.1016/j.jsg.2009.11.007.
4. Berryman, J.G. (2010), Poroelastic measurement schemes resulting in complete data sets for granular and other anisotropic porous media. LBNL-2914E. *International Journal of Engineering Sciences*, 48, 446–459.
5. Berryman, J.G., and A. Aydin (2010), Quasi-static analysis of elastic behavior for some systems having higher fracture densities. LBNL-3016E. *International Journal for Numerical and Analytical Methods in Geomechanics*, 34, 1687–1724.
6. Berryman, J.G., and S. Nakagawa (2010), Inverse problem in anisotropic poroelasticity: Drained constants from undrained ultrasound measurements. LBNL-3013E. *Journal of the Acoustical Society of America*, 127 (2), 720–729.
7. Berryman, J.G. (2010) Pore-fluid effects on seismic waves in vertically fractured earth with orthotropic symmetry. LBNL-4114E. *Geophysics*, 75 (6), T185–T200.
8. Bourg, I.C., and G. Sposito (2010), Connecting the molecular scale to the continuum scale for diffusion processes in smectite-rich porous media. LBNL-3045E. *Environmental Science & Technology*, 44 (6), 2085–2091; DOI: 10.1021/es903645a.
9. Bourg, I.C., F.M. Richter, J.N. Christensen, and G. Sposito (2010), Isotopic mass-dependence of metal cation diffusion coefficients in liquid water. LBNL-3046E. *Geochimica et Cosmochimica Acta*, 74 (8), 2249–2256.
10. Cortis, A, C.E. Puente, and B. Sivakumar (2010), Encoding hydrologic information via a fractal geometric approach and its extensions. *Stochastic Environmental Research and Risk Assessment*, 24(5), 625–632.
11. Cortis, A., and J.G. Berryman (2010), Frequency-dependent viscous flow in channels with fractal rough surfaces. LBNL-3602E. *Physics of Fluids*, 22, 053603.
12. Ewing, S.A., J.N. Christensen, S.T. Brown, R.A. Vancuren, S.S. Cliff, and D.J. DePaolo (2010), Pb isotopes as an indicator of the Asian contribution to particulate air pollution in urban California. *Environmental Science & Technology*, 44 (23), 8911–8916; DOI: 10.1021/es101450t.
13. Fantle, M.S., K.M. Maher, and D.J. DePaolo (2010), Isotopic approaches for quantifying the rates of marine burial diagenesis. *Reviews of Geophysics* , 48, RG3002; DOI: 10.1029/2009RG000306.
14. Ghose, S.K., G.A. Waychunas, T.P. Trainor, and P.J. Eng (2010), Hydrated goethite (α -FeOOH) (100) interface structure: Ordered water and surface functional groups. LBNL-4137E. *Geochimica et Cosmochimica Acta*, 74 (7), 1943–1953.
15. Gilbert, B., J.E. Katz, J.D. Denlinger, Y. Ying, R.W. Falcone and G.A. Waychunas (2010), Soft X-ray spectroscopy study of the electronic structure of oxidized and partially-oxidized magnetite nanoparticles. *Journal of Physical Chemistry C*, 114, 21994–22001.
16. Hinnell, A.C., T.P.A. Ferre, J.A. Vrugt, J.A. Huisman, S. Moysey, J. Rings, and M.B. Kowalsky (2010), Improved extraction of hydrologic information from geophysical data through coupled hydrogeophysical inversion. LBNL-3089E. *Water Resources Research*, 46, W00D40; DOI: 10.1029/2008WR007060).

17. Jun, Y.S., B. Lee, and G.A. Waychunas (2010), *In situ* observations of nanoparticle early development kinetics at mineral-water interfaces. *Environmental Science & Technology*, 44, 8182–8189.
18. Katz, J.E., B. Gilbert, X. Zhang, K. Attenkofer, and G.A. Waychunas (2010), Observation of transient iron(II) formation in dye-sensitized iron oxide nanoparticles by time-resolved X-ray spectroscopy. *J. Phys. Chem. Letters* 1, 1372–1376.
19. Kwon, K., K. Refson, and G. Sposito (2010), Surface complexation of Pb(II) by hexagonal birnessite nanoparticles. LBNL-4214E. *Geochimica et Cosmochimica Acta*, 74, 6731–6740.
20. Kwon, K., and G. Sposito (2010), Reactivity of biogenic manganese oxide for metal sequestration and photochemistry: LBNL-3685E. Computational solid state physics study. *Journal of the Mineralogical Society of Korea (in Korean)*, 23, 161–170.
21. Lee, V.E., D.J. DePaolo, and J.N. Christensen (2010), Uranium series comminution ages of continental sediments: Case study of a Pleistocene alluvial fan. LBNL-3832E. *Earth and Planetary Science Letters*, 296 (3–4), 244–254.
22. Masson, Y.J. and S.R. Pride (2010), Finite-difference modeling of Biot's poroelastic equations across all frequencies. LBNL-2808E. *Geophysics*, 75 (2); DOI:10.1190/1.3332589.
23. Mulvihill, M.J., S.E. Habas, I.J. La Plante, J. Wan, and T. Mokari (2010), The influence of size, shape, and surface coating on the stability of aqueous nanoparticle suspensions. LBNL-4124E. *Journal of Physical Chemistry*, 22 (18), 5251–5257.
24. Peña, J., K.D. Kwon, K. Refson, J.R. Bargar, and G. Sposito (2010), Mechanisms of nickel sorption by a bacteriogenic birnessite. LBNL-3657E. *Geochimica et Cosmochimica Acta*, 74, 3076–3089.
25. Rucci, A., D.W. Vasco, and F. Novali (2010). Fluid pressure arrival time tomography: Estimation and assessment in the presence of inequality constraints, with an application to a producing gas field at Krechba, Algeria. LBNL-3558E. *Geophysics*, 75 (6), 039; DOI:10.1190/1.3493504.
26. Silin, D., L. Tomutsa, S. Benson, and T. Patzek (2010), Microtomography and pore-scale modeling of two-phase fluid distribution. LBNL-3999E. *Transport in Porous Media*, 86 (2), 495–515; DOI: 10.1007/s11242-010-9636-2.
27. Vasco, D.W., A. Rucci, A. Ferretti, F. Novali, R. Bissell, P. Ringrose, A. Mathieson, and I. Wright (2010), Satellite-based measurements of surface deformation reveal fluid flow associated with the geological storage of carbon dioxide. LBNL-3018E. *Geophysical Research Letters*, 37, L03303; DOI: 10.1029/2009GL041544.
28. Vasco, D. (2010), On the propagation of a coupled saturation and pressure front. LBNL-4185E. *Water Resources Research*, 47, W03526; DOI:10.1029/WR97-865.
29. Vasco, D. (2010), On fluid flow in a heterogeneous medium under nonisothermal conditions. LBNL-4184E. *Water Resources Research*, 46; W12513; DOI:10.1029/2010WR009571.
30. Xu, M., X. Hu, K.G. Knauss, and S.R. Higgins (2010), Dissolution kinetics of calcite from 50–70°C: An atomic force microscopic study under near-equilibrium conditions. *Geochimica et Cosmochimica Acta*, 74, 4285–4297.
31. Zhang, H.Z., B. Chen, Y. Ren, G.A. Waychunas, and J.F. Banfield (2010), Response of nanoparticle structure to different types of surface environments: Wide-angle x-ray

scattering and molecular dynamics simulations. *Physical Review B*, 81 (12), Article 125444.

2009

Peer-Reviewed Journal Articles, Books, and Book Chapters for 2009

1. Bazin, D., X. Carpentier, I. Brocheriou, P. Dorfmuller, S. Aubert, C. Chappard, D. Thiaudiere, S. Reguer, G. Waychunas, P. Jungers, and M. Daudon, Revisiting the localization of Zn²⁺ cations sorbed on pathological apatite calcifications made through X-ray absorption spectroscopy. LBNL-2933E. *Biochimie*, 91, 1294–1300, 2009.
2. Berryman, J.G., Poroelastic measurement schemes resulting in complete data sets for granular and other anisotropic porous media. LBNL-2914E. *International Journal of Engineering Sciences*, 48, 446–459 (published online 2009), 2010.
3. Berryman, J.G., and A. Aydin, Quasi-static analysis of elastic behavior for some systems having higher fracture densities. LBNL-3016E. *International Journal for Numerical and Analytical Methods in Geomechanics* (in press, published online 2009), 2010.
4. Berryman, J.G., Aligned vertical fractures, HTI reservoir symmetry, and Thomsen seismic anisotropy parameters for polar media. LBNL-63659. *Geophysical Prospecting*, 57, 193–208, 2009.
5. Berryman, J.G., Frequency dependent thermal expansion in binary viscoelastic composites. LBNL-63655. *Mechanics of Materials*, 41, 463–480, 2009.
6. Berryman, J.G., Fluid effects on seismic waves in hard rocks with fractures and in soft granular media. LBNL-2041E. In: *Poro-Mechanics IV*, H.I. Ling, A. Smyth, and R. Betti, eds., *Proceedings of the Fourth Biot Conference on Poromechanics*, Columbia University, New York, New York, June 8–10, 2009, DESTech Publications, Lancaster, Pennsylvania, pp. 598–603, 2009.
7. Borg, L.E., A.M. Gaffney, C.K. Shearer, D.J. DePaolo, I.D. Hutcheon, T.L. Owens, E. Ramon, and G. Brennecka, Mechanisms for incompatible-element enrichment on the Moon deduced from the lunar basaltic meteorite Northwest Africa. *Geochimica et Cosmochimica Acta*, 73, 3963–3980. DOI: 03210.1016/j.gca.2009.03.039, 2009.
8. Bourg, I.C., and G. Sposito, Connecting the molecular scale to the continuum scale for diffusion processes in smectite-rich porous media. LBNL-3045E. *Environmental Science & Technology*, published online 2009 (DOI: 10.1021/es903645a) 2010.
9. Gilbert, B., R.K. Ono, K.A. Ching and C. S. Kim, The effects of nanoparticle aggregation processes on aggregate structure and metal uptake. *Journal of Colloid and Interface Science*, 339, 285–295, 2009.
10. Gilbert, B., C. Frandsen, E. Maxey and D. M. Sherman, Soft x-ray spectroscopy studies of the electronic structure of hematite nanoparticles. *Physical Review B*, 79, 035108 2009.
11. Kwon, K.D., K. Refson, and G. Sposito, On the role of Mn(IV) vacancies in the photoreductive dissolution of hexagonal birnessite. LBNL-2054E. *Geochimica et Cosmochimica Acta*, 73, 4142–4150, 2009.

12. Kwon, K.D., K. Refson, and G. Sposito, Zinc surface complexes on birnessite: A density functional theory study. LBNL-1553E. *Geochimica et Cosmochimica Acta*, 73, 1273–1284, 2009.
13. Lo, W.-C., G. Sposito, and E. Majer, Analytical decoupling of poroelasticity equations for acoustic-wave propagation and attenuation in a porous medium containing two immiscible fluids. *Journal of Engineering Mathematics*, 64, 219–235, 2009.
14. Lu, G., D.J. DePaolo, Q. Kang, and D. Zhang, Lattice Boltzmann simulation of snow crystal growth in clouds. *Journal of Geophysics Research*, 114, D07305, doi: 10.1029/2008JD011087, 2009.
15. Maher, K., C. I. Steefel, A.F. White, D.A. Stonestrom, The role of reaction affinity and secondary minerals in regulating chemical weathering rates at the Santa Cruz Soil Chronosequence, California. LBNL-1761E. *Geochimica et Cosmochimica Acta*, 73 (10), 2804–2831, 2009.
16. Navarre-Sitchler, A., C.I. Steefel, L. Yang, L. Tomutsa, and S.L. Brantley, Evolution of porosity and diffusivity associated with chemical weathering of a basalt clast. LBNL-1759E. *Journal of Geophysical Research*, 114, doi:10.1029/2008JF001060. 2009.
17. Nico, P.S., B.M. Kumfer, I.M. Kennedy, and C. Anastasio, Redox dynamics of mixed metal (Mn, Cr, and Fe) ultrafine particles. LBNL-811E. *Aerosol Science and Technology*, 43 (1), 60–70, 2009.
18. Nico, P. S., B.D. Stewart, and S. Fendorf, Incorporation of oxidized uranium into Fe (hydr)oxides during Fe(II) catalyzed remineralization. LBNL-2506E. *Environmental Science & Technology*, 43 (19), 7391–7396, 2009.
19. Spagnoli, D., B. Gilbert, G.A. Waychunas, and J. F. Banfield, Prediction of the effects of size and morphology on the structure of water around hematite nanoparticles. LBNL-2936E. *Geochimica & Cosmochimica Acta*, 73, 4023–4033, 2009.
20. Steefel, C.I., and K. Maher, Fluid-rock interaction: A reactive transport approach. LBNL-1798E. *Reviews in Mineralogy and Geochemistry*, 70 (1), 485–532, 2009.
21. Tokunaga, T. K., Hydraulic properties of adsorbed water films in unsaturated porous media. LBNL-1787E. *Water Resources Research*, 45, W06415, doi:10.1029/2009WR007734, 2009.
22. Tufano, K.J., S.G. Benner, K.U. Mayer, M.A. Marcus, P.S. Nico, and S. Fendorf , Aggregate-scale heterogeneity in iron (hydr)oxide reductive transformations. LBNL-2615E. *Vadose Zone Journal*, 8 (4), 1004–1012, 2009.
23. Vasco, D.W., Modelling broad-band poroelastic propagation using an asymptotic approach. LBNL-2807E. *Journal of Geophysics International*, 179, 299–318, 2009.
24. Vasco, D.W., and S.E. Minkoff, Modelling flow in a pressure-sensitive, heterogeneous medium. LBNL-2841E. *Journal of Geophysics International*, 179, 972–989, 2009.
25. Wan, J., Y. Kim, T.K. Tokunaga, Z. Wang, S. Dixit, C. Steefel, E. Saiz, M. Kunz, and N. Tamura, Spatially resolved U(VI) partitioning and speciation: Implications for plume scale behavior of contaminant U in the Hanford vadose zone. LBNL-1682E. *Environmental Science & Technology*, 43 (7), 2247–2253, 2009.
26. Watkins, J.M., D.J. DePaolo, C. Huber, and F.J. Ryerson, Isotope fractionation by diffusion of multi-atom chemical species in silicate liquids. *Geochimica et Cosmochimica Acta*, 73, 7341–7359, 2009.
27. Waychunas, G., Natural nanoparticle structure, properties and reactivity from X-ray studies. LBNL-2844E. *Powder Diffraction*, 24, 89–93, 2009.

2008

Peer-Reviewed Journal Articles, Books, and Book Chapters for 2008

1. Anwar, S., A. Cortis, and M. Sukop, Lattice Boltzmann simulation of solute transport in heterogeneous porous media with conduits to estimate macroscopic continuous time random walk model parameters. *Progress in Computational Fluid Dynamics*, 8 (1-4), 213-221, 2008.
2. Bazin, D., X. Carpentier, O. Traxer, D. Thiaudiere, A. Somogyi, S. Reguer, G. Waychunas, and M. Daudon, Very first tests on SOLEIL regarding the Zn environment in pathological calcifications made of apatite determined by X-ray absorption spectroscopy. LBNL-1735E. *Journal of Synchrotron Radiation*, 15, 506–509, 2008.
3. Benning, L.G., and G.A. Waychunas, Nucleation, growth, and aggregation of mineral phases: Mechanisms and kinetic controls. LBNL-1747E. Chapter 7 in: *Kinetics of Water-Rock Interaction*, S.L. Brantley, J D Kubicki and A F White, eds., pp. 259–334, Springer, New York, 2008.
4. Berryman, J.G., Elastic and transport properties in polycrystals of cracked grains: Cross-property relations and microstructure. LBNL-63502. *International Journal of Engineering Science*, 46, 500–512, 2008. doi:10.1190/1.2813433, 2008.
5. Bourg, I.C., G. Sposito, and A.C.M. Bourg, Modeling the diffusion of Na⁺ in compacted water-saturated Na-bentonite as a function of pore water ionic strength. LBNL-1781E. *Applied Geochemistry* 23, 3635–3641, 2008.
6. Bourg, I.C., and G. Sposito, Isotopic fractionation of noble gases by diffusion in liquid water: Molecular dynamics simulations and hydrologic applications. LBNL-63368. *Geochimica et Cosmochimica Acta*, 72, 2237–2247, 2008.
7. Brown, S.T., B.M. Kennedy , D.J. DePaolo, and W.C. Evans, Isotopic constraints on the chemical evolution of geothermal fluids, Long Valley, CA. LBNL-2411E. *GRC Transactions*, 32, 269–272, 2008.
8. Cervini-Silva, J., B. Gilbert, S. Fakra, S. Freidlich and J. F. Banfield., Decarboxylation and polymerization of catechol and formation of CeO₂ due to coupled redox and dissolution reactions at the surface of cerium(III) phosphate. *Geochimica et Cosmochimica Acta*, 72, 2454–2464, 2008.
9. Cochebin, B., L. Trotignon, O. Bildstein, C. Steefel, V. Lagneau, J. Van Der Lee, Intercomparison of predictions on a 2-D cementation experiment in porous medium. LBNL-809E. *Advances in Water Resources*, 31 (12), 1540–1551, 2008.
10. Deng, X., A. Verdaguer, T. Herranz, Ch.D. Weiss, H. Bluhm, and M. Salmeron, Surface chemistry of Cu in the presence of CO₂ and H₂O. *Langmuir*, 24 (17), 9474–9478, 2008.
11. DePaolo, D.J., and F.M. Orr, Geoscience research for our energy future. *Physics Today*, 61 (8), 46–51, 2008.
12. Erbs, J.J., B. Gilbert, and R.L. Penn, Influence of size on reductive dissolution of six-line ferrihydrite. *Journal of Physical Chemistry B*, 112, 12127–12133, 2008.
13. Finsterle, S., and M. B. Kowalsky, Joint hydrological-geophysical inversion for soil structure identification. LBNL-60088. *Vadose Zone Journal*, 7, 287–293, 2008.

14. Gaft, M., L. Nagli, G. Panczer, G. Waychunas, and N. Porat, The nature of unusual luminescence in natural calcite, CaCO_3 . LBNL-1734E. *American Mineralogist*, 93, 158–167, 2008.
15. Gilbert, B., Finite size effects on the real-space pair distribution function of nanoparticles. LBNL-1756E. *Journal of Applied Crystallography*, 41, 554–562, 2008.
16. Goodell, C., B. Gilbert, S. Weigand, H. Zhang and J. F. Banfield, The kinetics of the water adsorption driven structural transformation of ZnS nanoparticles. *Journal of Physical Chemistry C*, 112, 4791–4796, 2008.
17. Hausrath, E.M., A.K. Navarre-Sitchler, P.B. Sak, C.I. Steefel, and S.L. Brantley, Basalt weathering rates on Earth and the duration of liquid water on the plains of Gusev Crater, Mars. LBNL-829E. *Geology*, 36(1), 67–70, 2008.
18. Hopp, L., P.S. Nico, M.A. Marcus, and S. Peiffer, Arsenic and chromium partitioning in a podzolic soil contaminated by chromated copper arsenate. LBNL-353E. *Environmental Science & Technology*, 42(17), 6481–6486, 2008.
19. Kim, C.S., C.J. Lentini, and G.A. Waychunas, Associations between iron oxyhydroxide nanoparticle growth and metal adsorption/structural incorporation. LBNL-1788E. In: *Adsorption of Metals by Geomedia II*, M. Barnett and D. Kent, eds., Elsevier Developments in Earth & Environmental Sciences, 7, Chapter 6, pp.153–187, 2008.
20. Kwon, K. D., K. Refson, and G. Sposito, Defect-induced photoconductivity in layered manganese oxides: A density functional theory study. LBNL-63294. *Physical Review Letters*, 100 (146601), 2008.
21. Pride, S. R., E.G. Flekkey, and O. Orsjo, Seismic stimulation for enhanced oil recovery. LBNL-61828. *Geophysics*, 73 (5), doi:10.1190/1.2968090, 2008.
22. Soler, J.M., M. Boi, J.L. Mogollón, J. Cama, C. Ayora, P.S. Nico, N. Tamura, and M. Kunz, The passivation of calcite by acid mine water. Column experiments with $\text{Fe(III)}\text{-SO}_4\text{-H}^+$ and $\text{Fe(III)}\text{-Cl}\text{-H}^+$ solutions at pH 2. LBNL-955E. *Applied Geochemistry*, 23 (12), 3579–3588, 2008.
23. Teh, Y.A., E.A. Dubinsky, W.L. Silver and C.M. Carlson, Suppression of methanogenesis by dissimilatory Fe(III) -reducing bacteria in tropical rain forest soils: implications for ecosystem methane flux. *Global Change Biology*, 14, 413–422, 2008.
24. Tian, C., N. Ji, G. Waychunas, and Y.R. Shen, Interfacial structures of acidic and basic aqueous solutions. LBNL-1721E. *J. Amer. Chem. Soc.*, 130, 13033–13039, 2008.
25. Tokunaga, T. K., J. Wan, Y. Kim, S. R. Sutton, M. Newville, A. Lanzirotti, and W. Rao, Real-time x-ray absorption spectroscopy of uranium, iron, and manganese in contaminated sediments during bioreduction. LBNL-718E. *Environmental Science & Technology*, 42, 2839–2844, 2008.
26. Vasco, D. W., A. Ferretti, and F. Novali, Estimating permeability from quasi-static deformation: Temporal variations and arrival time inversion. LBNL-310E. *Geophysics*, 73 (6), 37–52, 2008.
27. Vasco, D. W., A. Ferretti, and F. Novali, Reservoir monitoring and characterization using satellite geodetic data: Interferometric synthetic radar observations from the Krechba field, Algeria. LBNL-308E. *Geophysics*, 73 (6), WA113-WA122, 2008.
28. Vasco, D. W., and H. Keers, Seismic imaging of reservoir flow properties: Resolving water influx and reservoir permeability. LBNL-63532. *Geophysics*, 73 (1), doi:10.1190/1.2789395, 2008.

29. Vasco, D.W., Modelling quasi-static poroelastic propagation using an asymptotic approach. LBNL-63547. *Geophysical Journal International*, 173, 1119–1135, 2008.
30. Vasco, D.W., Trajectory-based methods for modeling and characterization. LBNL-63531. In: Quantitative Information Fusion for Hydrological Sciences. C. Xing and T.-C. Jim Yeh, eds., Springer-Verlag, 79, 2008.
31. Vasco, D.W., Zeroth order inversion of transient head observations. LBNL-63537. *Water Resources Research*, 24 (2), 025013, 2008.
32. Waychunas, G.A., Y.-S. Jun, P. J. Eng, S. Ghose, and T. P. Trainor, Anion sorption topology on hematite: Comparison of arsenate and silicate. LBNL-61150. In: Adsorption of Metals by Geomedia II, M. Barnett and D. Kent, eds., Elsevier, Developments in Earth & Environmental Sciences, 7, Chapter 2, pp. 31–67, 2008.
33. Waychunas, G.A., H. Zhang, and B. Gilbert, Structure, chemistry, and properties of mineral nanoparticles. LBNL-1754E. *Elements*, 4, 381–387, 2008.
34. Xia, T., M. Kovochich, M. Liong, L. Madler, B. Gilbert, H. Shi, J. I. Yeh, J. I. Zink & A. E. Nel, Comparison of the mechanism of toxicity of zinc oxide and cerium oxide nanoparticles based on dissolution and oxidative stress properties. *ACS Nano Letters*, 2, 2121–2134, 2008.
35. Xu, T., Incorporation of aqueous reaction kinetics and biodegradation into TOUGHREACT: Application of a multi-region model to hydrobiogeochemical transport of denitrification and sulfate reduction. LBNL-61086. *Vadose Zone Journal*, doi: 10.2136/vzj.2006.0130305–315, 2008.
36. Yang, L., and C.I. Steefel, Kaolinite dissolution and precipitation kinetics at 22°C and pH 4. LBNL-830E. *Geochimica et Cosmochimica Acta*, 72(1), 99–116, 2008.
37. Zhang, H., B. Chen, J.F. Banfield, and G.A. Waychunas, Atomic structure of nanometer-sized amorphous TiO₂. LBNL-1722E. *Physical Review B*, 78, 214106, DOI: 10.1103/PhysRevB.78.214106, 2008.
38. Zhang, L., C. Tian, G.A. Waychunas, and Y.R. Shen, Structures and charging of alpha-alumina (0001)/water interfaces studies by sum-frequency vibrational spectroscopy. LBNL-1740E. *Journal of the American Chemical Society*, 130, 7686–7692, 2008.

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Peer-Reviewed Journal Articles, Books, and Book Chapters for 2007

1. Aciego, S., D.J. DePaolo, B.M. Kennedy, K.W.W. Sims, and M. Lamb (2007), Combining [³He] cosmogenic dating with U-Th/He eruption ages using olivine in basalt. *Earth and Planetary Science Letters*, 254, 288–302.
2. Berryman, J.G., Seismic waves in rocks with fluids and fractures. LBNL-62925. *Geophysical Journal International*, 171 (2), 954–974, 2007.
3. Berryman, J.G., and V. Grechka, Random polycrystals of grains containing cracks: Model of quasistatic elastic behavior for fractured systems. LBNL-61135. *Journal of Applied Physics*, 100 (Paper No. 113527), 2007.
4. Block, G., M.B. Rubin, J. Morris, and J.G. Berryman, Simulations of dynamic crack propagation in brittle materials using nodal cohesive forces and continuum damage

- mechanics in the distinct element code LDEC. LBNL-61404. *International Journal of Fracture*, 144, 131–147, 2007.
- 5. Bourg, I.C., and G. Sposito, Molecular dynamics simulations of kinetic isotope fractionation during the diffusion of ionic species in liquid water. LBNL-61833. *Geochimica et Cosmochimica Acta*, 71 (23), 5583–5589, 2007.
 - 6. Bourg, I.C., G. Sposito, and A.C.M. Bourg, Modeling the acid-base surface chemistry of montmorillonite. LBNL-62408. *Journal of Colloid and Interface Science*, 312 (2), 297–310, 2007.
 - 7. Bourg, I.C., G. Sposito, and A.C.M. Bourg, Modeling cation diffusion in compacted water-saturated Na-bentonite at low ionic strength. LBNL-63446. *Environmental Science and Technology* 41 (23), 8118–8122, 2007.
 - 8. Chen, B., B. Gilbert, H. Zhang, and J. Banfield, Mechanism of inhibition of nanoparticle growth and phase transformation by surface impurities. LBNL-63060. *Physical Review Letters*, 98 (10), 106103, 2007.
 - 9. DePaolo, D.J., and D. Weis (2007), Hotspot volcanoes and large igneous provinces. In: *Continental Scientific Drilling: A Decade of Progress and Challenges for the Future*, Harms, U. et al., ed., Springer-Verlag, 366pp.
 - 10. DePaolo, D.J., E.M. Stolper, and D.M. Thomas (2007), Scientific drilling in hotspot volcanoes. In: *McGraw-Hill Yearbook of Science and Technology 2007*, pp. 203–205.
 - 11. Fantle, M.S., and D.J. DePaolo (2007), Ca isotopes in carbonate sediment and pore fluid from ODP Site 807A: The $\text{Ca}^{2+}(\text{aq})$ -calcite equilibrium fractionation factor and calcite recrystallization rates in Pleistocene sediments. *Geochimica et Cosmochimica Acta*, 71, 2524–2546.
 - 12. Feineman, M.D., F.J. Ryerson, D.J. DePaolo, and T. Plank, Zoisite-aqueous fluid trace element partitioning with implications for subduction zone fluid composition. *Chemical Geology*, 239, 250–265, 2007.
 - 13. Fransson, A., C.-F. Tsang, J. Rutqvist, and G. Gustafson, A new parameter to assess hydromechanical effect in single-hole hydraulic testing and grouting. LBNL-801E. *International Journal of Rock Mechanics and Mining Sciences*, 44 (7), 1011–1021, 2007.
 - 14. Gilbert, B., G. Lu, and C.S. Kim, Stable nanoparticle clusters formed under environmentally relevant conditions. LBNL-60208. *Journal of Colloid and Interface Science*, 313, 152–159, 2007.
 - 15. He, Y. T., J. Wan, and T. K. Tokunaga, Kinetic stability of hematite nanoparticles: The effect of particle sizes. LBNL-63366. *J. Nanopart. Res.*, 10, 321–332, 2007.
 - 16. Keers, H., L.R. Johnson, and D. Vasco, W., Determination of porosity and saturation using seismic waveform inversion. *Studia Geophysica and Geodetica*, 51 (1), 119–140, 2007.
 - 17. Kennedy, B.M., and M.C. van Soest, Flow of mantle fluids through the ductile lower crust: Helium isotope trends. *Science*, 318, 1433–1436, 2007.
 - 18. Lee, J.-E., I. Fung, D.J. DePaolo, and C.C. Hening, Analysis of the global distribution of water isotopes using the NCAR atmospheric general circulation model. *Journal of Geophysical Research*, 112, D16306, doi:10.1029/2006JD007657, 2007.

19. Li, L., C.A. Peters, and M.A. Celia, Applicability of averaged concentrations in determining geochemical reaction rates in heterogeneous porous media. LBNL-63304. American Journal of Science, 307, 1146–1166, 2007.
20. Lo, W.-C., G. Sposito, and E. Majer, Low-frequency dilatational wave propagation through unsaturated porous media containing two immiscible fluids. Transport in Porous Media, 68, 91–105, 2007.
21. Masson, Y.J., and S.R. Pride, Poroelastic finite-difference modeling of seismic attenuation and dispersion due to mesoscopic heterogeneity. LBNL-61830. Journal of Geophysical Research, 112 (B03204), 2007.
22. Moreau, J. W., P. K. Weber, M. C. Martin, B. Gilbert, I. D. Hutcheon, and J. F. Banfield, Extracellular proteins limit the dispersal of biogenic nanoparticles. LBNL-62685. Science, 316 (5831), 1600–1603, 2007.
23. Sims, K.W.A., R.P. Ackert, Jr., F.C. Ramos, R.A. Sohn, A.T. Murrell, and D.J. DePaolo, (2007), Determining eruption ages and erosion rates of Quaternary basaltic volcanism from combined U-series disequilibria and cosmogenic exposure ages. Geology, 35, 471–474.
24. Steefel, C.I, Geochemical kinetics and transport. LBNL-62362. In: Kinetics of Water-Rock Interaction, S.L. Brantley, J.D. Kubicki, and A.F. White, eds., Springer, New York, pp. 545–589, 2007.
25. Tokunaga, T., J. Wan, A. Lanzirotti, S. R. Sutton, and M. Newville, Long-term stability of organic carbon-stimulated chromate reduction in contaminated soils, and its relation to manganese redox status. LBNL-62676. Environmental Science & Technology, 41 (12), 4326–4331, 2007.
26. Vasco, D.W., Invariance, groups, and non-uniqueness: The discrete case. LBNL-57367. Geophysical Journal International, 168, 473–490, 2007.
27. Vasco, D.W., Trajectory-based modeling of broadband electromagnetic wavefields. LBNL-61362. Geophysical Journal International, 168, 949–963, 2007.
28. Vasco, D.W., C. M. Puskas, R. B. Smith, and C. M. Meertens, Crustal deformation and source models of the Yellowstone volcanic field from geodetic data. LBNL-61514. Journal of Geophysical Research, 112, doi:10.1029/2006JB004641, 2007.
29. Wan, J. T. Tyliszczak, and T. K. Tokunaga, Organic carbon distribution, speciation, and elemental correlations within soil microaggregates: Applications of STXM microscopy and NEXAFS spectroscopy. LBNL-63422. Geochimica et Cosmochimica Acta, 71, 5439–5449, 2007.
30. Werner, M. L., P.S. Nico, M.A. Marcus, and C. Anastasio, Use of Micro-XANES to speciate of chromium in airborne fine particles in the Sacramento Valley. LBNL-62779. Environmental Science & Technology, 41 (14), 4914–4924, 2007.

Reports, 2007

1. Vasco, D.W., Unsaturated zone transport: An asymptotic approach. LBNL-56204. Lawrence Berkeley National Laboratory, Berkeley, CA. 2007.

